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A NOTE ON THE APPLICATION OF SCHWINGER'S VARIATIONAL PRINCIPLE TO DIRAC'S EQUATION OF THE ELECTRON.

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1. The Variational Principle.

Schwinger's variational principle has been used for a wide variety of problems involving wave motion in which it is desired to find the amplitude of a scattered wave in terms of the incident wave.* Schwinger's method makes use of the fact that the amplitude of the scattered wave satisfies a variational principle. We shall indicate this variational principle briefly.

Let us consider a vector space. We may define two different inner products, the Hermitian and symmetric inner product, in this vector space. The Hermitian inner product (a,b) of two vectors a and b is defined by the condition that

(1) $$(a,b) = \overline{(b,a)}$$

where the bar indicates the complex conjugate. The symmetric inner product is defined by the condition

(2) $$(a,b) = (b,a) \quad .$$

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* See, for example, Schwinger's unpublished nuclear physics notes, or the lectures of N. Marcuvitz in the notes "Recent Developments in the Theory of Wave Propagation", Inst. App. Math. and Mech., N.Y.U., 1949-50. The point of view of the present note is close to that of the latter set of notes.

If we work in a vector space with a Hermitian inner product, an operator K is said to be Hermitian if

(3) $$(a,Kb) = (Ka,b) \quad .$$

On the other hand, if we consider a space which has a symmetric inner product, an operator K is said to be symmetric if

(4) $$(a,Kb) = (Ka,b) \quad .$$

It must be remembered that though equations (3) and (4) have the same appearance, they refer to different inner products.

Let us consider a space with a Hermitian inner product. Let us also consider the equation

(5) $$a = Ky$$

for the unknown vector y where K is a Hermitian operator and a is a given vector. We define the real number λ by

(6) $$\lambda = \frac{1}{(y,a)} = \frac{1}{(a,y)} \quad .$$

(The second equation follows from equation (5) together with the fact that K is Hermitian.) Also, we define the functional $\lambda\{v\}$ by

(7) $$\lambda\{v\} = \frac{(v,Kv)}{(v,a)(a,v)} \quad .$$

It is easily seen that

(8) $$\lambda\{y\} = \lambda \quad .$$

The variational principle used by Schwinger states that <u>$\lambda\{v\}$ has as its stationary value the value λ</u>. Thus to find λ one need only find the stationary value of $\lambda\{v\}$.

From (8) it is seen that if v approximates y to the first order then $\lambda\{v\}$ approximates $\lambda\{y\} = \lambda$ to the second order. This fact may be used to find λ to a high degree of accuracy.

A similar variational principle is valid if we work in a space with a symmetric inner product, and if the operator K is symmetric. In this case, however, λ is generally complex.

For the purpose of treatment of scattering problems, a generalization of the above variational principle is used. Let us again consider a vector space with a Hermitian inner product and consider a pair of equations

$$(9) \qquad \begin{cases} a = Ky \\ a' = K'y' \end{cases}$$

where K and K' are Hermitian adjoint operators which by definition satisfy the condition

$$(10) \qquad (K'u,v) = (u,Kv)$$

for any two vectors u and v. If $K' = K$, K is a Hermitian operator. It can be shown from (10) that

$$(11) \qquad (a',y) = (y',a)$$

which is called the <u>reciprocity theorem</u>. Let us define a number $\tilde{\lambda}$ by

$$(12) \qquad \tilde{\lambda} = \frac{1}{(y',a)} = \frac{1}{(a',y)}$$

and the functional $\tilde{\lambda}\{v,v'\}$ by

$$(13) \qquad \tilde{\lambda}\{v,v'\} = \frac{(v',Kv)}{(v',a)(a',v)} = \frac{(K'v',v)}{(v',a)(a',v)}$$

so that

$$\tilde{\lambda}\{y,y'\} = \tilde{\lambda} \quad . \tag{14}$$

It can be shown that $\tilde{\lambda}\{v,v'\}$ is stationary for independent variations of v and v' about the values y and y' respectively and that, therefore, from (14), the stationary value of $\tilde{\lambda}\{v,v'\}$ is $\tilde{\lambda}$.

A similar statement holds if the symmetric inner product is used. In this case K' is said to be the symmetric adjoint operator of K if K' and K are related by (10).

2. Schwinger's Application of the Variational Principle to Scattering Problems.

It will be convenient to introduce a notation for operators. The elements of the vector space in which we are interested will be functions of the coordinates, collectively denoted by the vector x, and other variables, collectively denoted by γ. An operator A which operates on functions of these variables will be denoted by $A^{x,\gamma}$. Hence if $f(x,\gamma)$ is an element of the vector space, the vector which results when the operator A operates on it is $A^{x,\gamma}f(x,\gamma)$. Frequently it is useful to consider operators as being integral operators with suitable kernels which may be symbolic functions, such as the δ-functions of Dirac. We shall define the kernel $A(x,\gamma;x',\gamma')$ by

$$A^{x,\gamma}\, f(x,\gamma) = \int A(x,\gamma;x',\gamma')\, f(x',\gamma')dx'\, d\gamma' \tag{15}$$

the integration being taken over the entire range of values of x and γ. The integration over γ is to be interpreted as a summation, if γ takes on discreet values only. The condition that the operator A is symmetric can be expressed by means of the kernel as

(16) $$A(x,\gamma;x',\gamma') = A(x',\gamma';x,\gamma) \quad .$$

Likewise the condition that A is a Hermitian operator can be expressed by the relation

(17) $$A(x,\gamma;x',\gamma') = \overline{A(x',\gamma';x,\gamma)} \quad .$$

In scattering problems one is interested in solving differential equations of the form

(18) $$H^{x,\gamma}\chi(x,\gamma;E) = E\chi(x,\gamma;E)$$

subject to boundary conditions to be discussed shortly. Here $H^{x,\gamma}$ is a Hermitian differential operator, E is a real number which is considered fixed, and $\chi(x,\gamma;E)$ is a function of the coordinates denoted by the vector x and other variables collectively denoted by γ. One may regard the problem of finding the solution $\chi(x,\gamma;E)$ of (18) as that of finding the eigenfunctions for a fixed eigenvalue E.

In scattering problems the operator $H^{x,\gamma}$ is given as

(19) $$H^{x,\gamma} = H_0^{x,\gamma} + q^{x,\gamma}$$

where $H_0^{x,\gamma}$ is a function of derivatives with respect to the coordinates and can be written $H_0^{x,\gamma} = H_0^{\gamma}(\frac{\partial}{\partial x})$, and

$q^{x,\gamma}$ is a function of x, which we may write as $q^{x,\gamma} = q^{\gamma}(x)$, which will be assumed to vanish for $|x| \geq r_o$.

This last condition on $q^{\gamma}(x)$ is somewhat severe and for many purposes may be replaced by the less severe one that $q^{\gamma}(x)$ approach zero sufficiently rapidly for large values of $|x|$.

In this manner we have placed some restrictions on the nature of the operator $H^{x,\gamma}$ insofar as it operates with respect to the variable x.

It is now possible to specify boundary conditions on the functions $\chi(x,\gamma;E)$. The boundary conditions are specified in the following way: the solution $\chi(x,\gamma;E)$ of the differential equation (18) is to be such that it can be written in the form

$$(20) \qquad \chi(x,\gamma;E) = \chi_{in}(x,\gamma;E) + \chi_{sc}(x,\gamma;E)$$

where the function $\chi_{in}(x,\gamma;E)$ (which is called the incident wave) is a <u>given</u> solution of the differential equation

$$(21) \qquad H_o^{x,\gamma}\chi_{in}(x,\gamma;E) = E\,\chi_{in}(x,\gamma;E)$$

and where the function $\chi_{sc}(x,\gamma;E)$ (which is called the scattered wave) is to be found so as to behave like an outgoing spherical wave for large values of $|x|$. These boundary conditions are sufficient to determine $\chi(x,\gamma;E)$ uniquely. For many problems in which E is a multiple

eigenvalue of the operator $H_o^{x,\gamma}$ it is useful to label the functions $\psi_{in}(x,\gamma;E)$ by an additional set of variables.

The function $\chi_{sc}(x,\gamma;E)$ satisfies the equation

$$(22) \qquad (E - H_o^{x,\gamma})\chi_{sc}(x,\gamma;E) = q^{x,\gamma}\chi(x,\gamma;E) \quad .$$

Using an appropriate inverse operator $[E - H_o^{x,\gamma}]^{-1}$, equation (22) is seen to be equivalent to the equation

$$(23) \qquad \chi_{sc}(x,\gamma;E) = [E - H_o^{x,\gamma}]^{-1}\, q^{x,\gamma}\chi(x,\gamma;E) \quad .$$

The inverse operator $[E - H_o^{x,\gamma}]^{-1}$ is to be expressed in terms of an integral operator using for the kernel an influence function which gives χ_{sc} the proper behavior for large values of $|x|$.

Having chosen such an influence function we desire to express χ_{sc} for large values of $|x|$ as a sum of terms of the form $\theta_i(x,\gamma;E)T_i(E)$, i.e.,

$$(24) \qquad \chi_{sc}(x,\gamma;E) = \sum_i \theta_i(x,\gamma;E)\, T_i(E)$$

$$|x| \to \infty \quad ,$$

where $\theta_i(x,\gamma;E)$ are appropriately chosen spherical waves and the functions $T_i(E)$ are "amplitudes" which are inner products to which one can apply the second variational principle discussed in Part I of the present note.

The function $\chi(x,\gamma;E)$ is identified with the vector y of equation (9), the operator K is identified with the operator $q^{x,\gamma} - q^{x,\gamma}[E - H_o^{x,\gamma}]\, q^{x,\gamma}$, and the vector a

is identified with the function $q^{x,\gamma}\chi_{in}(x,\gamma;E)$. The first of equations (9) is merely a form of equation (23). The operator K' is taken as the symmetric adjoint or Hermitian adjoint operator of K. The vector a' will be so chosen that the function $T_1(E)$ is the inner product (a',y). Thus $[T_1(E)]^{-1}$ is identified with λ. The vector y' is then taken as the solution of the second of equations (9). It is seen that the manner of decomposition of χ_{sc} into spherical waves given by (24) determines how a' shall be chosen.

3. Application of the Variational Principle to the Scattering of the Dirac Electron.

A. Dirac's Equation for the Electron.

The above concepts can be illustrated by considering the scattering of the Dirac electron. Schwinger has treated the problem somewhat in his nuclear physics notes. However, he does not use an explicit form for the inverse operator $[E - H_0^{x,\gamma}]^{-1}$. In the present note we shall make use of such an explicit form in terms of an integral operator and show what quantities are to be identified with a' and y'.

In Dirac's theory of the electron, the elements of the vector space are functions $f(x,\gamma)$ of the coordinates denoted collectively by the vector x, and of a variable γ which is restricted to four values which may

be taken as 1,2,3,4. These functions are called spinor components. The Hermitian inner product of $f(x,\gamma)$ and $g(x,\gamma)$ is given by $\sum_{\gamma=1}^{4} \int \overline{f(x,\gamma)}\, g(x,\gamma)dx$ and the symmetric inner product by $\sum_{\gamma=1}^{4} \int f(x,\gamma)\, g(x,\gamma)dx$. An operator $A^{x,\gamma}$ may be represented by an integral operator with a kernel $A(x,\gamma;x',\gamma')$ given by the definition (15). For some purposes such a representation of the operator is useful.

Dirac's wave equation for the electron in an electromagnetic field is

$$(25) \qquad \frac{i\,\partial\,\psi(x,\gamma;t)}{\partial t} = H^{x,\gamma}\,\psi(x,\gamma;t)$$

where

$$(26) \qquad H^{x,\gamma} = \sum_{j=1}^{3} \alpha_j^{\gamma}\; i\left(\frac{\partial}{\partial x_j} + e\,A_j(x)\right) + e\,\phi(x) - m\beta^{\gamma}$$

Here α_j^{γ} and β^{γ} are Hermitian operators which operate with respect to the γ variable only. They satisfy the following commutation relations

$$(27) \qquad \begin{cases} \alpha_j^{\gamma}\,\alpha_i^{\gamma} + \alpha_i^{\gamma}\,\alpha_j^{\gamma} = 2\,\delta_{ij}\,I^{\gamma} \\ \beta^{\gamma}\,\alpha_j^{\gamma} + \alpha_j^{\gamma}\,\beta^{\gamma} = 0 \\ (\beta^{\gamma})^2 = I^{\gamma} \end{cases}$$

where I^{γ} is the identity operator.

The operators α_j^{γ} , β^{γ} can be expressed as integral operators with kernels $\alpha_j(\gamma,\gamma')$, $\beta(\gamma,\gamma')$ which are the well-known Dirac matrices.

In the expression (26) we have taken $\hbar = c = 1$. The mass of the electron is m and its charge is e. The functions $A_i(x)$ and $\phi(x)$ are the vector and scalar potentials of an electromagnetic field and are taken as real.

We shall look for solutions of equation (25) which can be written as

$$(28) \qquad \psi(x,\gamma;t) = e^{-iEt}\chi(x,\gamma;E)$$

so that equation (25) leads to

$$(29) \qquad H^{x,\gamma}\chi(x,\gamma;E) = E\,\chi(x,\gamma;E) \quad .$$

This equation is of the form (18) with $H^{x,\gamma}$ given by (26).

For the case of the Dirac electron we define $H_o^{x,\gamma}$ as

$$(30) \qquad H_o^{x,\gamma} = i\sum_{j=1}^{3} \alpha_j^{\gamma}\frac{\partial}{\partial x_j} - m\,\beta^{\gamma}$$

and $q^{x,\gamma}$ by

$$(31) \qquad q^{x,\gamma} = e\sum_{j=1}^{3}\alpha_j^{\gamma} A_j(x) + e\,\phi(x)$$

where $A_j(x)$ and $\phi(x)$ are to vanish for $|x| \geq r_o$ so that

$$q^{x,\gamma} \equiv q^{\gamma}(x) \equiv 0 \quad \text{for} \quad |x| \geq r_o \quad .$$

We have thus specified $H_o^{x,\gamma}$ and $q^{x,\gamma}$ of equation (19).

B. <u>The Incident Wave.</u>

As in the general procedure of Part II of the present note we shall write

$$\chi = \chi_{in} + \chi_{sc} \quad .$$

We require that χ_{in} be a solution of

$$H_o^{x,\gamma} \chi_{in}(x,\gamma;E) = E \chi_{in}(x,\gamma;E)$$

where $H_o^{x,\gamma}$ is given by (30). Suitable solutions are the "spinor plane wave" solutions which have the form

$$(32) \qquad \chi_{in}(x,\gamma;E) = \chi(\gamma;E,\eta,\tau)\ e^{i|k|(\eta x)}$$

where η is a unit vector which specifies the direction of propagation, (ηx) is the inner product of the vectors x and η, and $|k|$ is the absolute value of the momentum and is given by the relation

$$(33) \qquad |k|^2 = E^2 - m^2 \quad ,$$

The quantities $\chi(\gamma;E,\eta,\tau)$ are functions of their arguments. Here τ is a variable which is restricted to two values which may be taken as +1 and -1. The significance of τ is that, in the non-relativistic approximation, it represents the z component of the spin.

By substituting (32) into the equation $H_o^{x,\gamma}\chi_{in} = E\chi_{in}$ it is seen that the functions $\chi(\gamma;E,\eta,\tau)$ satisfy the following equation

$$(34) \qquad \left\{ E + |k| \sum_{j=1}^{3} \alpha_j^{\gamma} \eta_j + \beta^{\gamma} m \right\} \chi(\gamma;E,\eta,\tau) = 0 \quad .$$

For the purpose of the present note, it is not necessary to give an explicit form for the functions $\chi(\gamma;E,\eta,\tau)$; these functions can be found in textbooks. However, it

will be useful to indicate the orthogonality properties of the functions. These orthogonality relations are

$$\sum_{\gamma} \overline{\chi(\gamma;E,\eta,\tau)}\, \chi(\gamma;E,\eta,\tau') = \delta_{\tau\tau'}$$

(35)

$$\sum_{\gamma} \overline{\chi(\gamma;-E,\eta,\tau)}\, \chi(\gamma;E,\eta,\tau') = 0 \quad ,$$

also

(35a)
$$\sum_{\tau} \chi(\gamma;E,\eta,\tau)\, \overline{\chi(\gamma';E,\eta,\tau)} + \sum_{\tau} \chi(\gamma;-E,\eta,\tau)\, \overline{\chi(\gamma';-E,\eta,\tau)} = \delta(\gamma,\gamma') \quad .$$

From the above relations it can be shown that any function $f(\gamma)$ of γ can be expressed as a linear combination of the functions

$\chi(\gamma;E,\eta,+1)$, $\chi(\gamma;E,\eta,-1)$, $\chi(\gamma;-E,\eta,+1)$, and $\chi(\gamma;-E,\eta,-1)$

for fixed values of E and η .

C. The Integral Representation of the Operator $[E - H_0^{x,\gamma}]^{-1}$: The Integral Equation for the Scattered Wave.

Through expression (32) we have given acceptable functions χ_{in}. We wish now to set up the integral equation for χ_{sc} corresponding to equation (23). We shall express $[E - H_0^{x,\gamma}]^{-1}$ as an integral operator such that χ_{sc} as given by (23) behaves like an outgoing spherical wave for large values of $|x|$.

For this purpose let us consider the differential

equation

(36) $$(E - H_o^{x,\gamma})\, f(x,\gamma) = k(x,\gamma) \quad ,$$

where $f(x,\gamma)$ is subject to the boundary condition that for large values of $|x|$ $f(x,\gamma)$ is to behave like an outgoing spherical wave. The solution of (36) can be written

(37) $$f(x,\gamma) = (E - H_o^{x,\gamma})^{-1}\, k(x,\gamma)$$
$$= \sum_{\gamma'} \int g(x,\gamma;x',\gamma')\, k(x',\gamma')dx'$$

provided $k(x,\gamma)$ dies out sufficiently rapidly for large values of $|x|$. The second of equations (37) expresses the inverse operator $(E - H_o^{x,\gamma})^{-1}$ as an integral operator. The boundary condition on $f(x,\gamma)$ will determine the form of the influence function $g(x,\gamma;x',\gamma')$. We shall then have the desired integral representation for the inverse operator $(E - H_o^{x,\gamma})^{-1}$.

The influence function satisfies the following equation

(38) $$[E - H_o^{x,\gamma}]g(x,\gamma;x',\gamma') = \delta(x - x')\, \delta(\gamma,\gamma') \quad .$$

Let us now consider the operator $[E - H_o^{x,\gamma}]$. Then from the commutation rules (27) for α_i^γ , β^γ one has

(39) $$[E + H_o^{x,\gamma}][E - H_o^{x,\gamma}] = [E - H_o^{x,\gamma}][E + H_o^{x,\gamma}]$$
$$= (E^2 - m^2 + \nabla^2) \qquad = (|k|^2 + \nabla^2) \quad .$$

In fact it was the requirement that equation (39) hold, which led Dirac to the commutation laws (27).

We shall now consider a solution of the differential equation

$$(40)\quad (E^2 - m^2 + \nabla_x^2)\, s(x,x') \equiv (|k|^2 + \nabla_x^2)\, s(x,x') = \delta(x - x') \quad .$$

(The subscript x on the operator ∇^2 indicates that the differentiations are to be carried out on the variable x rather than x'.)

Any solution s(x,x') of equation (40) can be used to form a solution of equation (38).

From (39) and (40) one has

$$(41)\quad [E - H_o^{x,\gamma}][E + H_o^{x,\gamma}]s(x,x')\delta(\gamma,\gamma') = \delta(x-x')\delta(\gamma,\gamma').$$

Hence a solution $g(x,\gamma;x',\gamma')$ of (38) is

$$(42)\qquad g(x,\gamma;x',\gamma') = (E + H_o^{x,\gamma})\, s(x,x')\, \delta(\gamma,\gamma') \quad .$$

This method of obtaining influence functions for the Dirac operator is a well-known one. A solution $s_r(x,x')$ of (40) which leads to a solution $f(x,\gamma)$ which is an outgoing wave is

$$(43)\qquad s_r = - \frac{e^{i|k||x-x'|}}{4\pi|x-x'|} \quad .$$

The influence function g_r obtained using s_r is in explicit form

(44) $$g_r(x,\gamma;x',\gamma') =$$

$$- \left\{ \frac{-[\,|k|\,|x-x'|+i]}{|x-x'|^2} \sum_{i=1}^{3} \alpha_i(\gamma,\gamma')(x_i-x_i') \right.$$

$$\left. - m\beta(\gamma,\gamma') + E\delta(\gamma,\gamma') \right\} \frac{e^{i|k|\,|x-x'|}}{4\pi|x-x'|} \quad .$$

The function g_r represents an outgoing wave because the time factor is e^{-iEt} (see (28)). Thus the solution of (36) representing an outgoing wave is

(45) $$f(x,\gamma) = \sum_{\gamma'} \int g_r(x,\gamma;x',\gamma')\, k(x',\gamma')dx' \quad .$$

For large values of $|x|$, $f(x,\gamma)$ takes the form

(46) $$f(x,\gamma) = - \frac{e^{i|k|\,|x|}}{4\pi|x|} \sum_{\gamma'} \left\{ [E\delta(\gamma,\gamma') \right.$$

$$- |k| \sum_{i=1}^{3} \alpha_i(\gamma,\gamma')\,\eta_{1i}$$

$$\left. - m\beta(\gamma,\gamma')] \int e^{-i|k|(x',\eta_1)}\, k(x',\gamma')dx' \right\} \quad .$$

Here η_1 is a unit vector with components η_{1i} defined by

(47) $$x = |x|\,\eta_1$$

and is thus the direction of observation. It is thus seen that $f(x,\gamma)$ behaves like an outgoing spherical wave for large values of $|x|$, as desired.

Having found the form of the inverse operator $[E - H_o^{x,\gamma}]^{-1}$ which satisfies the boundary conditions we can express χ_{sc} in terms of χ by

(48) $$\chi_{sc}(x,\gamma) = \sum_{\gamma'} \int g_r(x,\gamma;x',\gamma') q^{x',\gamma'} \chi(x',\gamma') dx' \quad .$$

The factor $q^{x',\gamma'}\chi(x',\gamma')$ in the integrand means that the function $\lambda(x,\gamma)$ which results from applying the operator $q^{x,\gamma}$ on $\chi(x,\gamma)$ is to have its arguments x and γ replaced by x' and γ' respectively. Equation (48) is the desired integral equation for χ_{sc}.

D. <u>The Asymptotic Equation for the Scattered Wave.</u>

For large values of $|x|$, the integral equation for χ_{sc} becomes

(49) $$\chi_{sc}(x,\gamma) = - \frac{e^{i|k||x|}}{4\pi|x|} \sum_{\gamma'} \Big\{ [E\delta(\gamma,\gamma') - |k| \sum_{i=1}^{3} \alpha_i(\gamma,\gamma')\eta_{1i} - m\beta(\gamma,\gamma')] \int e^{-i|k|(x',\eta_1)} q^{x',\gamma'} \chi(x',\gamma') dx' \Big\} .$$

We wish now to write (49) in a form similar to (24) in order that the variational principle may be used as described in Part II of this note. Looking at the integral in (49) we see that the integral is very nearly an inner product of the function formed by the operator $q^{x,\gamma}$ acting on a spinor plane wave and the function $\chi(x,\gamma)$, provided one introduces as a factor the function $\chi(\gamma;E,\eta,\tau)$ which was used in the definition of the spinor plane wave (see (32)). This line of thought motivates our use of the identity

$$(50)\quad [E\delta(\gamma,\gamma') - |k| \sum_{i=1}^{3} \alpha_i(\gamma,\gamma')\eta_{1i} - m\beta(\gamma,\gamma')]$$

$$= 2E \sum_{\tau} \chi(\gamma;E,\eta_1,\tau)\overline{\chi(\gamma';E,\eta_1,\tau)} \quad .$$

Before showing how this identity is used, we shall verify it. We use the orthogonality relation

$$(33a)\quad \sum_{\tau} \chi(\gamma;E,\eta,\tau)\overline{\chi(\gamma';E,\eta,\tau)} + \sum_{\tau} \chi(\gamma;-E,\eta,\tau)\overline{\chi(\gamma';-E,\eta,\tau)} = \delta(\gamma,\gamma')$$

and equation (32), which we write as

$$(51)\quad \sum_{\gamma'} H_o(\gamma,\gamma')\chi(\gamma';E,\eta,\tau) = E\chi(\gamma;E,\eta,\tau)$$

where

$$(52)\quad H_o(\gamma,\gamma') = -|k| \sum_{j=1}^{3} \alpha_j(\gamma,\gamma')\eta_j - m\beta(\gamma,\gamma') \quad .$$

Hence from (33a)

$$(53)\quad H_o(\gamma,\gamma') = \sum_{\gamma''} H_o(\gamma,\gamma'')\delta(\gamma'',\gamma')$$

$$= E\left\{\sum_{\tau} \chi(\gamma;E,\eta,\tau)\overline{\chi(\gamma';E,\eta,\tau)} - \sum_{\tau} \chi(\gamma;-E,\eta,\tau)\overline{\chi(\gamma';-E,\eta,\tau)}\right\} \quad .$$

The operator $E\delta(\gamma,\gamma') - |k| \sum_{j=1}^{3} \alpha_j(\gamma,\gamma')\eta_j - m\beta(\gamma,\gamma')$ may be written $E\delta(\gamma,\gamma') + H_o(\gamma,\gamma')$. Multiplying (33a) by E and adding the resulting equation to (53), one obtains

$$(54)\quad E\delta(\gamma,\gamma') + H_o(\gamma,\gamma') = 2E \sum_{\tau} \chi(\gamma;E,\eta,\tau)\overline{\chi(\gamma';E,\eta,\tau)}$$

which is the identity (50).

Now we shall show that we have χ_{sc} expressed in the form (24) for large values of $|x|$, when we use the identity (50) in (49). If the incident wave part of the function $\chi(x,\gamma)$ has the direction η' and the value of τ is τ', we shall denote $\chi(x,\gamma)$ by $\chi(x;\gamma;E,\eta',\tau')$. We proceed to define the "spinor spherical wave" $\theta(x,\gamma;E,\eta,\tau)$ by

(55) $$\theta(x,\gamma;E,\eta,\tau) = -\frac{E\ e^{i|k||x|}}{2\pi|x|}\ \chi(\gamma;E,\eta,\tau) \quad .$$

The spinor spherical wave is analogous to the spinor plane wave (32). Furthermore, we define $T(E;\eta,\tau;\eta',\tau')$ by

(56) $$T(E;\eta,\tau;\eta',\tau') =$$
$$\sum_{\gamma'}\int \overline{\chi(\gamma';E,\eta,\tau)}\ e^{-i|k|(x',\eta)}q^{x',\gamma'}\ \chi(x',\gamma';E,\eta',\tau')dx'.$$

Then the integral equation for χ_{sc} takes the form for large $|x|$,

(57) $$\chi_{sc}(x,\gamma) \equiv \chi_{sc}(|x|\eta_1,\gamma)$$
$$= \sum_{\tau} \theta(x,\gamma;E,\eta_1,\tau)\ T(E;\eta_1,\tau;\eta',\tau') \quad .$$

The scattered wave may be regarded as the sum of two spinor spherical waves, each being characterized by a different value of τ. The function $T(E;\eta_1,\tau_1;\eta_2;\tau_2)$ may be regarded as the amplitude of the spinor spherical wave in the direction η_1 and with $\tau = \tau_1$ when the incident spinor plane wave has as its direction of propagation η_2 and its value of τ is τ_2. We have therefore obtained

χ_{sc} in the desired form (24), where $T(E;\eta,\tau;\eta',\tau')$ is an inner product to which a variational principle can be applied.

E. Application of the Variational Principle.

In order to show how the second variational principle discussed in Part I may be used to find the amplitudes $T(E;\eta,\tau;\eta',\tau')$ we need only show what quantities are to be identified with the quantities appearing in equation (9). We carry out this identification in accordance with the procedure discussed in Part II.

Let us first consider $T(E;\eta,\tau;\eta',\tau')$ as being the symmetric inner product of two vectors. According to the general formalism of Part II of this note, we identify $\chi(x,\gamma;E,\eta',\tau')$ with the vector y of equation (9). We see that the vector a' is to be identified with $\overline{q^{x,\gamma}\,\chi(\gamma;E,\eta,\tau)}\ e^{-i|k|(x,\eta)}$, using the fact that $q^{x,\gamma}$ is a Hermitian operator.

The other identifications with the quantities of equation (9) can now be made easily. The operator K is identified with $q^{x,\gamma} - q^{x,\gamma}[E - H_o^{x,\gamma}]^{-1}q^{x,\gamma}$ and the vector a with $q^{x,\gamma}\chi(\gamma;E,\eta',\tau')e^{i|k|(x,\eta')}$ in accordance with the general procedure outlined in Part II.

In order to write the integral equation corresponding to the first of equations (9) in a convenient form, we shall write $q^{x,\gamma}$ and $[E - H_o^{x,\gamma}]^{-1}$ as integral operators with appropriate kernels. The kernel of the integral

operator corresponding to $q^{x,\gamma}$ is written

$$(58) \quad q(x,\gamma;x',\gamma') = e \sum_{j=1}^{3} a_j(\gamma,\gamma')\, A_j(x)\, \delta(x - x') + e\phi(x)\, \delta(x - x') \quad .$$

It is to be noted that

$$(59) \qquad \overline{q(x',\gamma';x,\gamma)} = q(x,\gamma;x',\gamma') \quad ,$$

since $q^{x,\gamma}$ is a Hermitian operator.

The equation corresponding to the first of equations (9) becomes in this notation

$$(60) \quad \sum_{\gamma'} \int q(x,\gamma;x',\gamma')\, \chi(\gamma';E,\eta',\tau')\, e^{i|k|(x',\eta')} dx'$$
$$= \sum_{\gamma'} \int \Big\{ q(x,\gamma;x',\gamma') - \sum_{\gamma''} \int q(x,\gamma;x'',\gamma'') \sum_{\gamma'''} \int g_r(x'',\gamma'';x''',\gamma''')\, q(x''',\gamma''';x',\gamma')\, dx''\, dx''' \Big\}\, \chi(x',\gamma';E,\eta',\tau')\, dx' \quad .$$

The integral equation (60) is merely a rewriting of equation (48), where we have used χ_{in} given by (32). The curly brackets contain the kernel of the integral operator $K^{x,\gamma}$.

To find the function Λ corresponding to the vector y' we shall write down the integral equation corresponding to the second equation (9). The symmetric adjoint operator $K'^{x,\gamma}$ may be written as an integral operator whose kernel is the transpose of the kernel of the integral operator corresponding to $K^{x,\gamma}$. Accordingly, the integral equation for Λ is

$$(61) \quad \sum_{\gamma'} \int \overline{q(x,\gamma;x',\gamma')}\ \overline{\mathcal{T}(\gamma';E,\eta,\tau)}\ e^{-i|k|(x',\eta)} dx'$$

$$= \sum_{\gamma'} \int \Big\{ \overline{q(x,\gamma;x',\gamma')} - \sum_{\gamma''} \int \overline{q(x,\gamma;x'',\gamma'')} \sum_{\gamma'''}$$

$$\int g_s(x'',\gamma'';x''',\gamma''')\ \overline{q(x''',\gamma''';x',\gamma')}\ dx''\ dx''' \Big\} \cdot$$

$$\cdot\ \Lambda(x',\gamma';E,\eta,\tau)\ dx'$$

where

$$(62) \qquad g_s(x,\gamma;x',\gamma') = g_r(x',\gamma';x,\gamma) \quad .$$

Just as the integral equation (60) for $\chi(x,\gamma;E,\eta,\tau)$ was derived from the differential equation

$$(63) \qquad H^{x,\gamma}\chi(x,\gamma;E,\eta,\tau) = E\,\chi(x,\gamma;E,\eta,\tau)$$

together with appropriate boundary conditions, the integral equation (61) for $\Lambda(x,\gamma;E,\eta,\tau)$ can be derived from a differential equation with certain boundary conditions. We shall write down the differential equation and boundary conditions and sketch the derivation of equation (61) from these.

The differential equation satisfied by Λ is

$$(64) \qquad \overline{H}^{x,\gamma}\Lambda(x,\gamma;E,\eta,\tau) = E\,\Lambda(x,\gamma;E,\eta,\tau)$$

so that Λ is an eigenfunction of $\overline{H}$. The boundary condition on Λ is that it is to be expressed as the sum of an incident wave Λ_{in} and a scattered Λ_{sc} such that Λ_{in} satisfies

(65) $\overline{H}_o^{x,\gamma}\Lambda_{in}(x,\gamma;E,\eta,\tau) = E\Lambda_{in}(x,\gamma;E,\eta,\tau)$

and Λ_{sc} behaves like the spherical wave $\frac{e^{ik|x|}}{|x|}$ for large values of $|x|$.

We take as a suitable solution Λ_{in} of (65) the function $\overline{\chi}_{in}$ where χ_{in} is given by (32). The function Λ_{sc} as can be shown from (64), satisfies the equation

(66) $(E - \overline{H}_o^{x,\gamma})\Lambda_{sc} = \overline{q^{x,\gamma}}\ \Lambda$

which can be written as the integral equation

(67) $\Lambda_{sc} = (E - \overline{H}_o^{x,\gamma})^{-1}\ \overline{q^{x,\gamma}}\ \Lambda$

where the inverse operator $(E - \overline{H}_o^{x,\gamma})^{-1}$ is represented by an integral operator with a suitable kernel. In a derivation similar to that for g_r, this kernel can be shown to be g_s defined by (62). Equation (61) is merely a rewriting of (67) using the function Λ_{in} described above.

Having considered the case where $T(E;\eta,\tau;\eta',\tau')$ is a symmetric inner product, we shall now discuss the case in which this amplitude is considered a Hermitian inner product of the two vectors $q^{x,\gamma}\chi(\gamma;E,\eta,\tau)e^{i|k|(\eta,x)}$ and $\chi(x,\gamma;E,\eta',\tau')$. The identification of the vectors a, and y and of the operator K are as before in the case of the symmetric inner product. The vector a' is now identified with $q^{x,\gamma}\chi(\gamma;E,\eta,\tau)e^{i|k|(\eta,x)}$; the operator K' which is the Hermitian conjugate of K is taken as an

integral operator whose kernel is the complex conjugate of the transposed kernel of the integral operator which represents K. The vector y' is identified with the function $\Omega(x,\gamma;E,\eta,\tau)$ which satisfies the following integral equation which corresponds to the second of equations (9).

$$\sum_{\gamma'} \int q(x,\gamma;x',\gamma')\,\chi(\gamma';E,\eta,\tau)\,e^{i|k|(\eta,x')}dx' \tag{68}$$

$$= \sum_{\gamma'} \int \Big\{ q(x,\gamma;x',\gamma') - \sum_{\gamma''} \int q(x,\gamma;x'',\gamma'')$$

$$\sum_{\gamma'''} \int g_t(x'',\gamma'';x''',\gamma''')\, q(x''',\gamma''';x',\gamma')\, dx''\, dx''' \Big\}$$

$$\Omega(x',\gamma';E,\eta,\tau)dx'$$

where

$$g_t(x,\gamma;x',\gamma') = \overline{g_r(x',\gamma';x,\gamma)} \tag{69}$$

$$= -\Big\{ \frac{[|k|\,|x-x'|-i]}{|x-x'|^2} \sum_{i=1}^{3} a_i(\gamma,\gamma')(x_i - x_i')$$

$$- m\,\beta(\gamma,\gamma') + E\delta(\gamma,\gamma') \Big\} \frac{e^{-i|k|\,|x-x'|}}{4\pi|x-x'|} \quad .$$

We can express $\Omega(x,\gamma;E,\eta,\tau)$ as a solution of a differential equation with suitable boundary conditions. We shall sketch the method by which the integral equation (68) may be obtained from the differential equation with the appropriate boundary conditions.

The function $\Omega(x,\gamma;E,\eta,\tau)$ satisfies the differential equation

$$H^{x,\gamma}\Omega(x,\gamma;E,\eta,\tau) = E\Omega(x,\gamma;E,\eta,\tau) \tag{70}$$

so that Ω, like χ, is an eigenfunction of $H^{x,\gamma}$. However, the function Ω has different boundary conditions than χ. The boundary condition on Ω is that it should be expressed as the sum of an incident part Ω_{in} and a "concentrating" part Ω_{con}. The function Ω_{in} satisfies

$$(71) \qquad H_o^{x,\gamma}\Omega_{in}(x,\gamma;E,\eta,\tau) = E\,\Omega_{in}(x,\gamma;E,\eta,\tau)$$

and is taken to be χ_{in} as given by (32). The function Ω_{con} is specified by the condition that Ω_{con} is to behave like an <u>inwardly</u> moving spherical wave for large values of $|x|$. The equation for Ω_{con} is

$$(72) \qquad (E - H_o^{x,\gamma})\Omega_{con} = q^{x,\gamma}\Omega \quad .$$

Equation (72) can also be written

$$(73) \qquad \Omega_{con} = [E - H_o^{x,\gamma}]^{-1}\, q^{x,\gamma}\,\Omega \quad .$$

Using the boundary condition that Ω_{con} represent an inward moving spherical wave for large values of $|x|$, the inverse operator $[E - H_o^{x,\gamma}]^{-1}$ can be expressed an an integral operator with the function g_t defined by (69) as kernel. Equation (68) is then simply another form of the equation (73) using the integral operator representation of the inverse operator. It might be noted that g_t is the solution of equation (38) expressed in the form (42) when the solution s of (40) is taken to be

$$s_t = - \frac{e^{-i|k|\,|x-x'|}}{4\pi|x-x'|}$$

instead of s_r given by (43).